

Fact Sheet

FREZCHEM: A Chemical–Thermodynamic Model for Aqueous Solutions at Subzero Temperatures

PROBLEM

Complex interactions exist between solute concentrations and the freezing process. The freezing points of aqueous solutions are lowered by the presence of solutes. When solutions freeze, the ice formation excludes solutes, concentrating them in the unfrozen brines, which, in turn, further lowers the freezing points of the brines.

A number of chemical–thermodynamic models for aqueous electrolyte solutions have been developed in recent years, but only one (Spencer–Møller–Weare) deals explicitly with aqueous solutions at subzero temperatures. A working model would be extremely useful for geochemists and geophysicists interested in the complex interactions between solutes and the freezing process.

SOLUTION

We have developed a FORTRAN version, called FREZCHEM, of the Spencer–Møller–Weare model. FREZCHEM is a chemical–thermodynamic model for aqueous electrolyte solutions at subzero temperatures. It predicts the chemical composition and unfrozen water of aqueous solutions between -60°C and $+25^{\circ}\text{C}$ at atmospheric pressure (0.101325 MPa).

FREZCHEM includes two reaction pathways: 1) freezing at variable temperature and fixed total water, and 2) evaporation at variable water and fixed temperature. Activity coefficients and the activity of water are calculated using Pitzer equations, which are valid to high solution ionic strengths (about 20 mol/kg). Fifteen chloride and sulfate salts of sodium, potassium, calcium, and magnesium are included in the model.

Predicted and experimental measurements of solute molalities and the unfrozen water fractions during seawater freezing are in good agreement. At -50°C , 0.3% of seawater remains unfrozen, with 99.7% of sodium and 95.5% of chloride having precipitated into one of four salts.

PRODUCTS AVAILABLE

- FORTRAN source code for the FREZCHEM computer model is available from Dr. Giles M. Marion.
- Marion, G.M., and S.A. Grant (1994) FREZCHEM: A chemical–thermodynamic model for aqueous solutions at subzero temperatures. USA Cold Regions Research and Engineering Laboratory, Special Report 94-18.
- Mironenko, M.V., S.A. Grant, G.M. Marion, and R.E. Farren (1997) FREZCHEM2: A chemical–thermodynamic model for electrolyte solutions at subzero temperatures. USA Cold Regions Research and Engineering Laboratory, CRREL Report 97-5.

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